The Lagrangian ice microphysics code LCM within EULAG: Basic overview and selected application examples

S. Unterstraßer

Outline

1) Introduction to LCM: overview, physics, strategy, benefits

2) Applications: contrails and natural cirrus

3) Optimisation of simulation particle number

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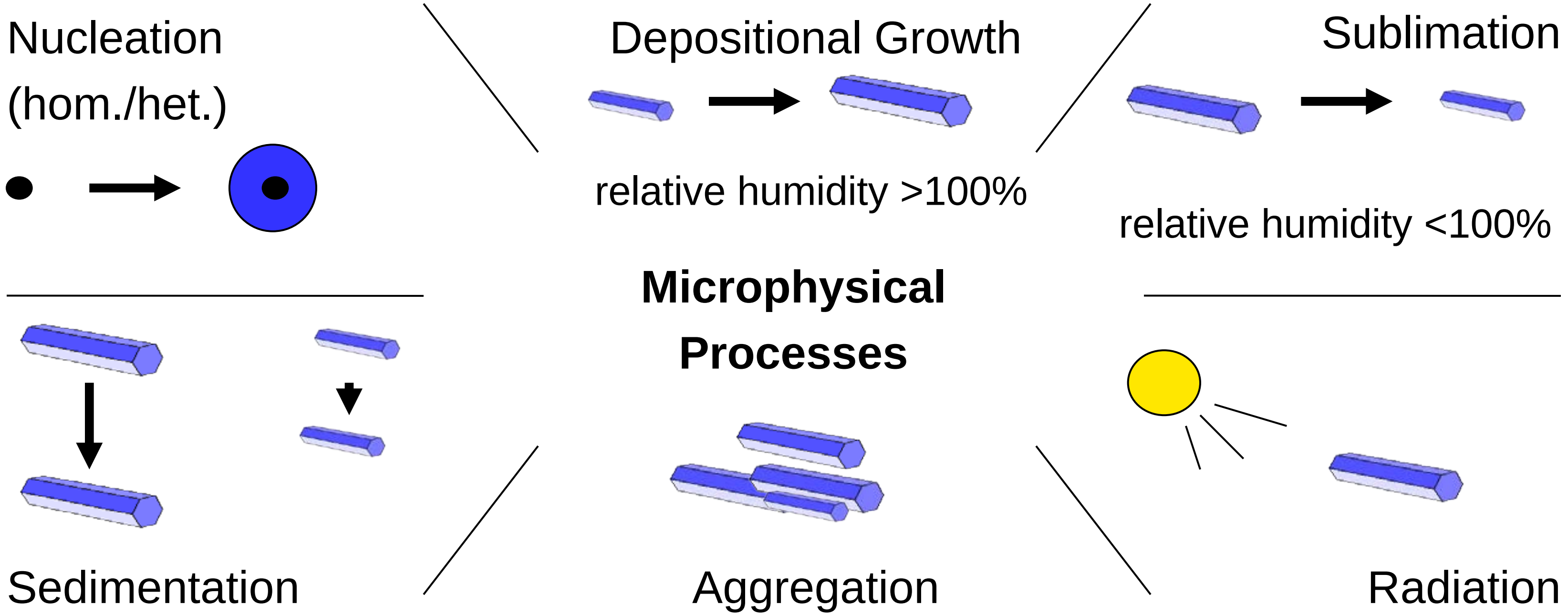
1) **Introduction to LCM: overview, physics, strategy, benefits**
2) Applications: contrails and natural cirrus
3) Optimisation of simulation particle number

Particle based approach =
Lagrangian microphysics =
Superdroplet method

Overview of ice microphysical processes



LCM module: overview

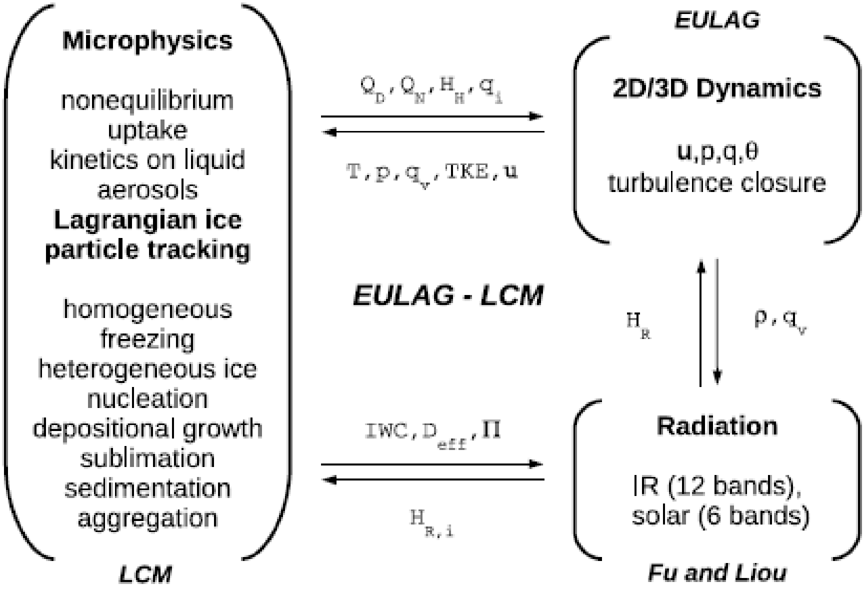


Figure 1. Schematic overview of the DLR EULAG-LCM model system. The LCM (Lagrangian Cirrus Module) can also be coupled to other dynamical core and radiation models, provided the interfaces for the exchange of model variables are similar.

Sölch & Kärcher, 2010, QJRMS

LCM module: physics

explicit aerosol and ice microphysics:

- non-equlibrium growth of supercooled aerosol particles (solution droplets of sulphuric acid H_2S0_4 and water H_20) + their homogeneous freezing;
  starts at RHi around 150%

- heterogeneous ice nucleation of ice nuclei (immersion/deposition mode);
  Threshold RHi depends on IN, but often smaller than for homogeneous freezing

- deposition/sublimation including ventilation, Kelvin and kinetic regime corrections and optionally radiative surface fluxes

LCM module: physics

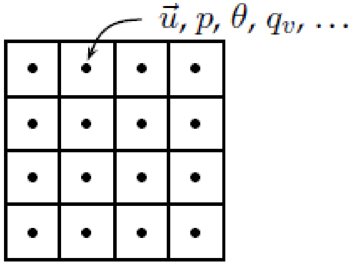
explicit aerosol and ice microphysics:

- sedimentation
- aggregation by gravitational settling
- advection including subgrid scale turbulence
- several ice crystal habit options (plates, bullet rosettes, spheres, hexagonal columns, aggregates)

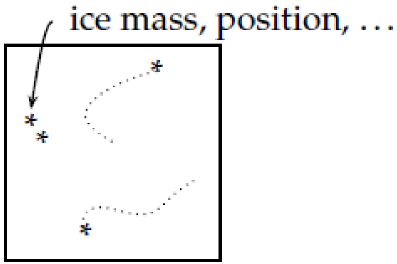
LCM module: strategy

- Lagrangian approach for ice phase: each simulation particle (SIP) represents m_{sim} identical ice crystals.

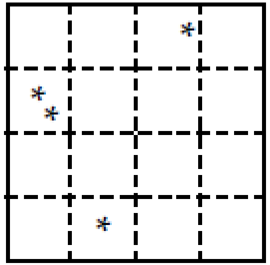
- Eulerian approach for all other quantities:
  water vapor, aerosol concentrations
  (spectrally resolved)



- SIPs have discrete position xp, yp, zp
  SIP carry information on ice crystal mass, habit, origin, turbulent particle velocity, m_{sim}



LCM module: strategy



- Attribution of SIPs to grid box for coupling with EULAG:
  - 1 to 1 relation
  - Any SIP affects one GB
  - SIPs use grid point values of EULAG (interpolation optionally)
- Coupling
  - water vapor, latent heat, aerosol for nucleation
  - density potential temperature (ice mass + water vapour corrected air density)

LCM module: processes

- Nucleation
  - subcycling of timestep, each small timestep SIPs are potentially generated.
  - a SIP is generated if more than m_{min} real ice crystal form ($m_{sim} > m_{min}$). *Note the difference to the superdroplet approach where a simulation particle changes its status from aerosol to cloud droplet and no new simulation particles are generated*

- Advection
  - Solve transport equation, where particle velocity is sum of
    - EULAG wind
    - sedimentation fall speed
    - auto-correlated subgrid scale turbulent fluctuations

LCM module: processes

- Deposition and sedimentation
  - solved individually for each SIP

- Aggregation
  - only by differential sedimentation
  - no „lateral“ collisions, no turbulence enhancement; probably not relevant for ice clouds
  - Throw away information on horizontal position, keep information on vertical position
  - pairwise collision testing of nearby SIPs
    sort SIPs by zp; costs O(n log n), where n is the number of SIP in a GB

LCM module: benefits

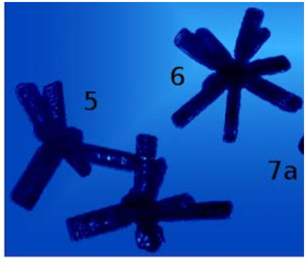
Lagrangian advection treatment

Deposition: Ice crystal size distributions evolve freely

Sedimentation: Straight-forward inclusion in advection equation

Aggregation: collisions explicitly resolved; SIPs carry information on collision history

Analysis of ice crystal trajectories



Outline

1) Introduction to LCM: overview, physics, strategy, benefits

2) **Applications: contrails and natural cirrus**

3) Optimisation of simulation particle number

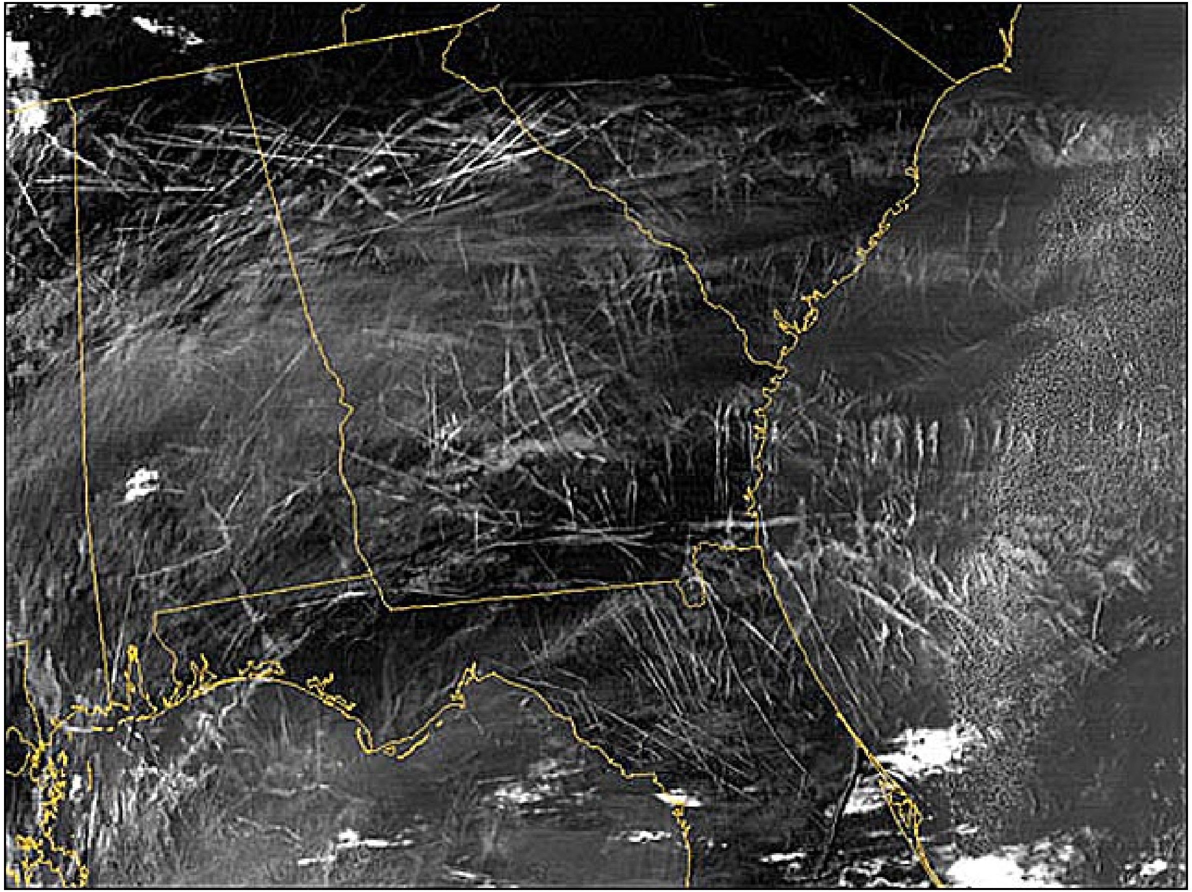
Application

Climate impact of aviation is assessed at my home institute DLR Oberpfaffenhofen.

Contrails are the major climate forcing of aviation

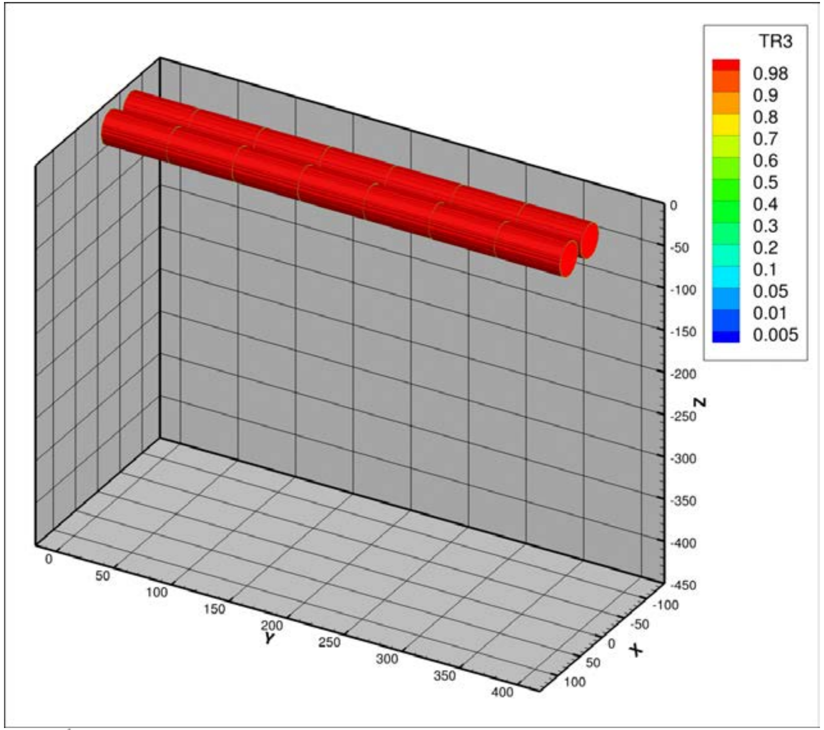
Applications of LCM focus on contrails and their interaction with natural cirrus

Motivation for contrail research



- see left image
- Supersaturation common feature of upper tropospheric air

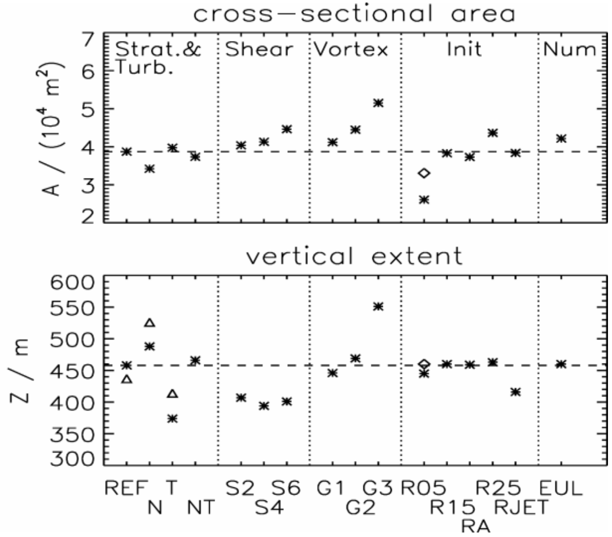
Application: young contrail (t < 5min)



- Two aspects are important:
  ice microphysics and
  wake vortex dynamics
- 3D simulation with 80e6 grid points and 160e6 SIPs and 10000 time steps
- covers first 5 minutes behind aircraft

Application: young contrail (t < 5min)

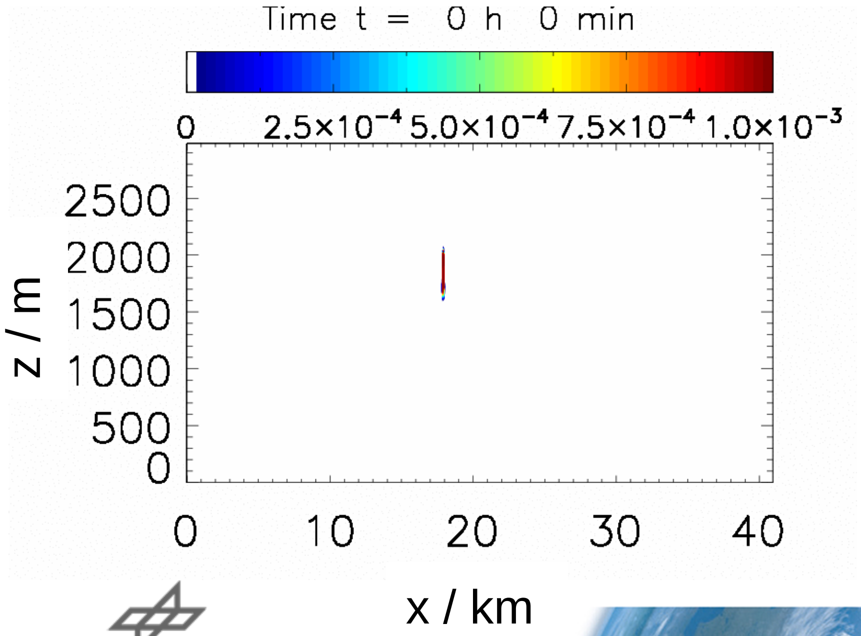
- Summary of sensitivity analyses
- Lagrangian approach is not prohibitive in terms of computing power



Dimension of aircraft exhaust plumes at cruise conditions: effect of wake vortices.
S.Unterstrasser, R. Paoli, I. Sölch, C. Kühnlein, T. Gerz, ACP, 2014

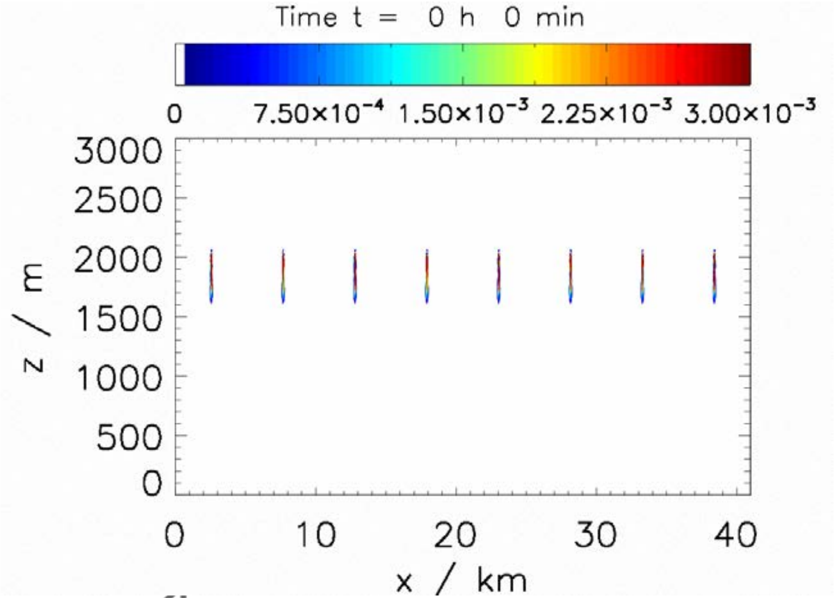
Application: contrail to cirrus transition

Evolution of a single contrail in a supersaturated layer with background vertical wind shear over 10 hours.



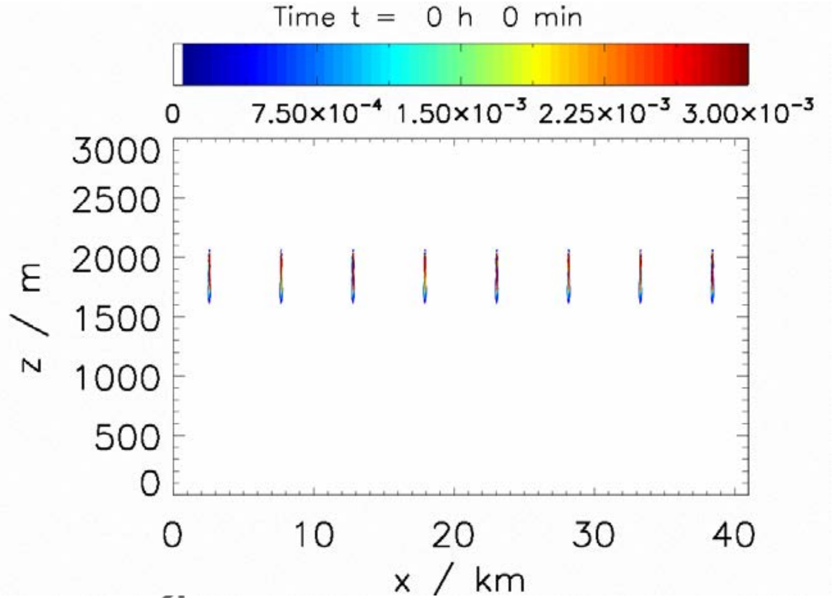
Application: contrail to cirrus transition

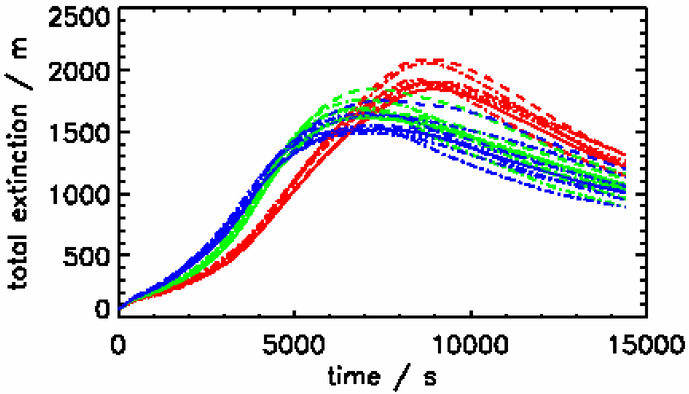
Evolution of eight contrails in a supersaturated layer with background vertical wind shear over 4 hours.



Application: contrail to cirrus transition

Evolution of eight contrails in a supersaturated layer with background vertical wind shear over 4 hours.





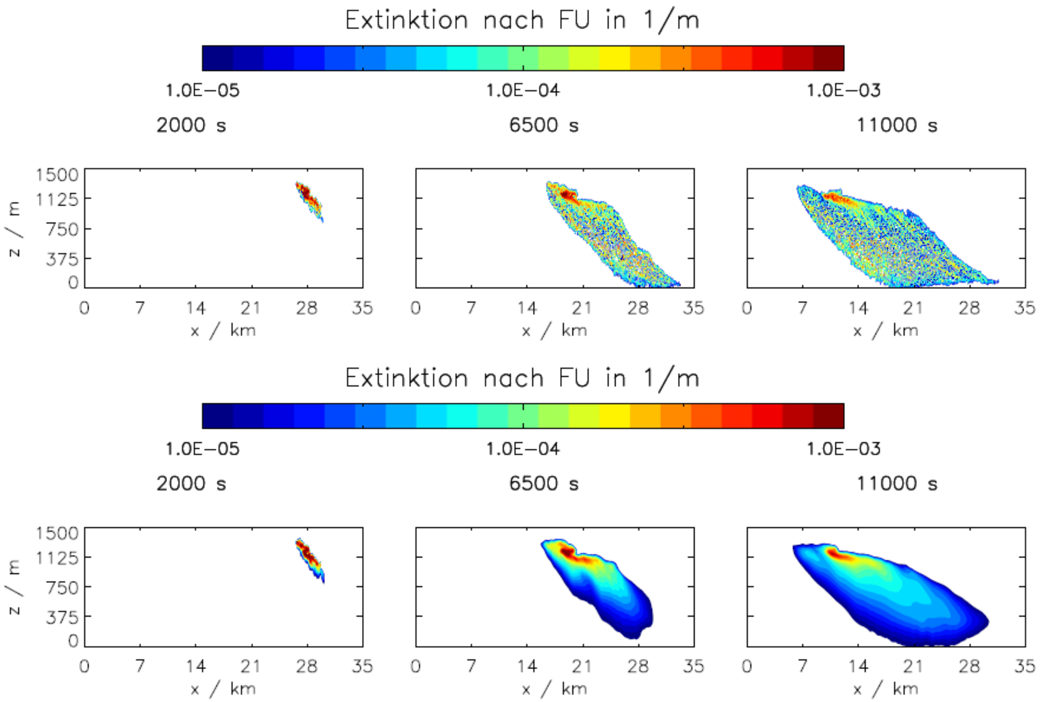
Analyse each contrail instance separately by introducing a memory-efficient flag variable

Application: comparison with BULK scheme

Comparison of

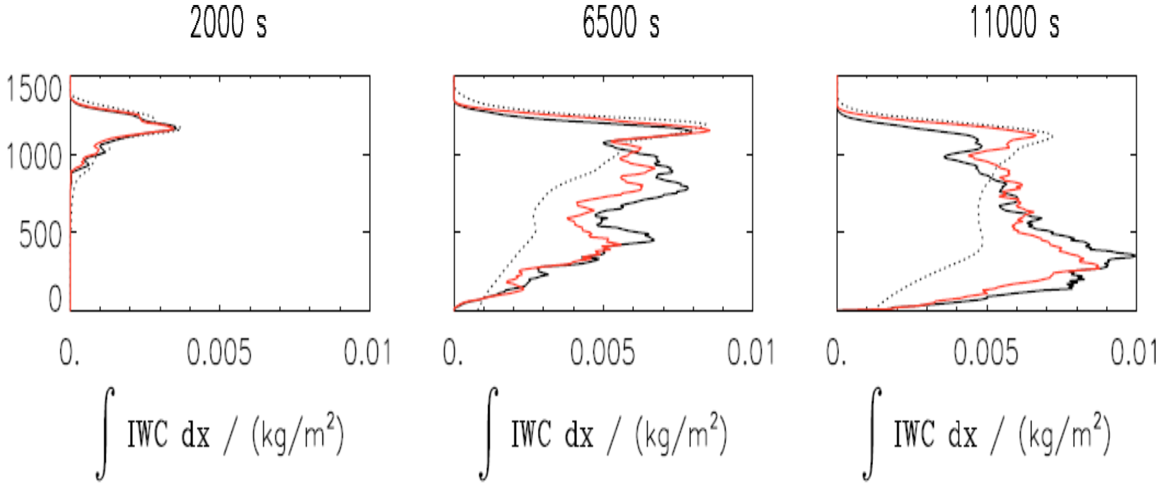
LCM

BULK; two moments (Spichtinger & Gierens)

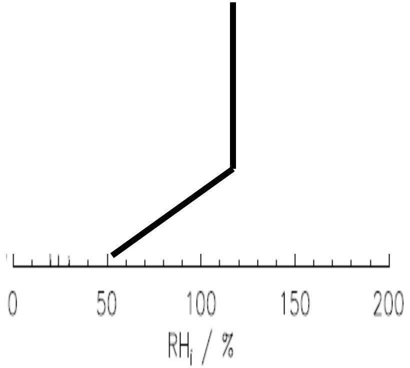


Application: comparison with BULK scheme

Comparison of **LCM** (solid) and **BULK** (dotted): Vertical distribution



Humidity profile

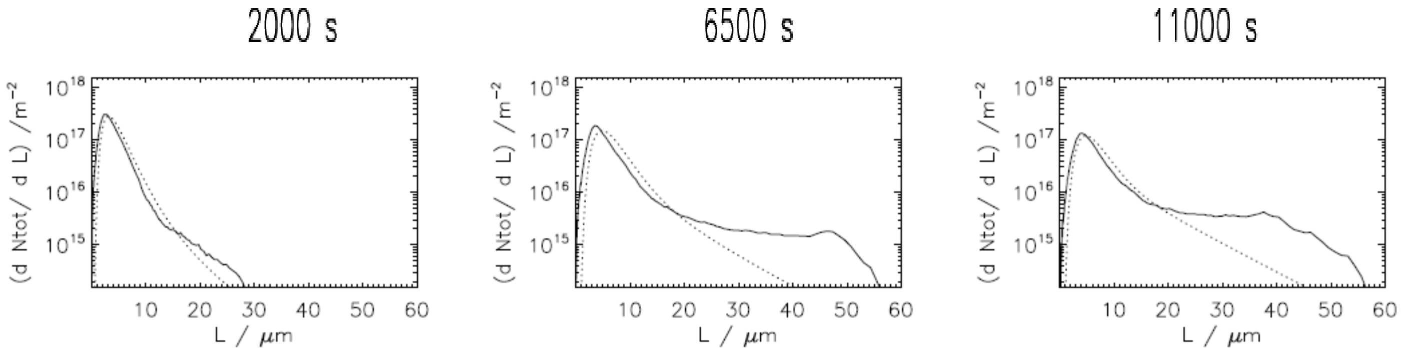


Solid black: original LCM implementation;

Solid red: LCM implementation with sedimentation parametrization as in BULK

Application: comparison with BULK scheme

Comparison of **LCM** (solid) and **BULK** (dotted): size distribution

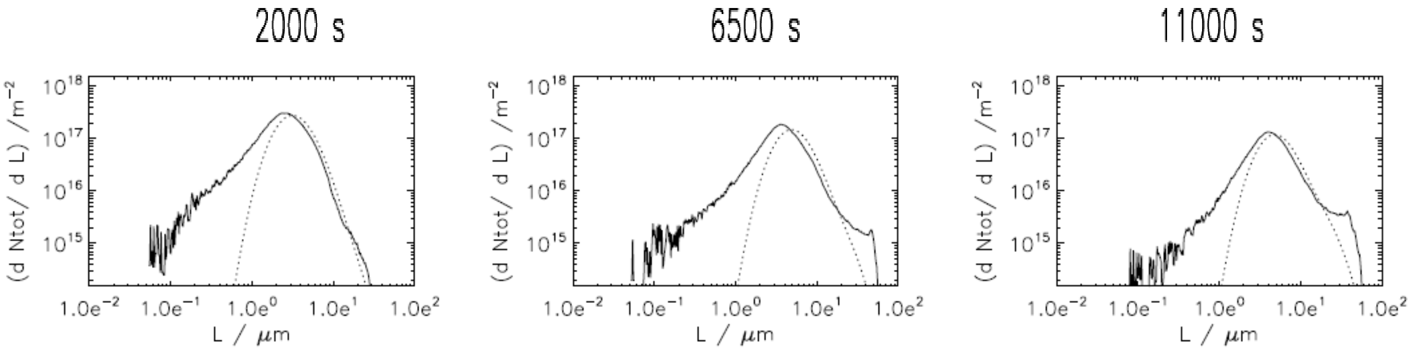


Maximum crystal sizes in fall streak better captured in LCM

Application: comparison with BULK scheme

Comparison of **LCM** (solid) and **BULK** (dotted): size distribution

now log-scale



Broadening of size distribution due to Kelvin effect (Lewellen, JAS, 2012) in LCM: “Spectral ripening“ important in slowly ascending air.

Outline

1) Introduction to LCM: overview, physics, strategy, benefits

2) Applications: contrails and natural cirrus

3) **Optimisation of simulation particle number (described in Unterstrasser & Sölch, 2014, GMD)**

Convergence issue

Memory and computing time scales linearly with number of SIPs.
How many SIPs are necessary to describe the microphysical processes sufficiently well? When do we reach physical convergence?

We found that deposition and sedimentation are well resolved with less than 50 SIP per GB

Threshold depends also on the smoothness of the background fields

Nucleation highly non-linear process, large number of SIPs is necessary.
Recent improvements reduces the SIP numbers

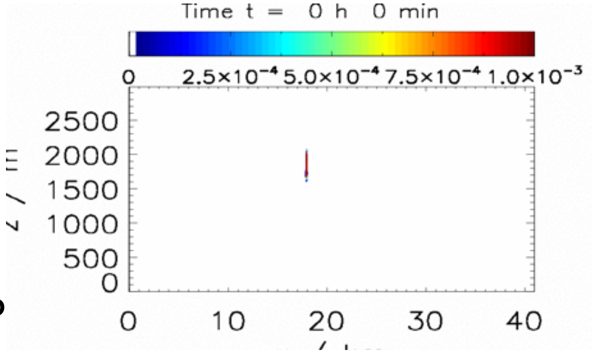
Convergence issue: Deposition and sedimentation

Simulation with prescribed ice cloud and nucleation switched off

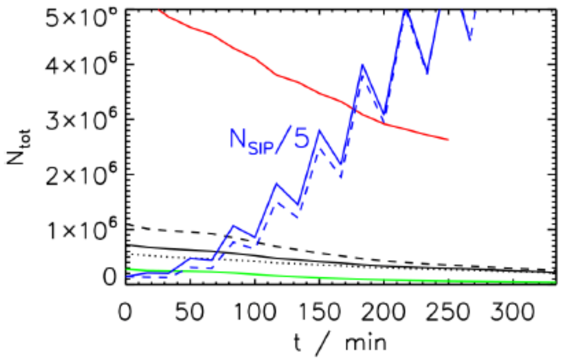
Variation of number of simulation particles N_{tot}

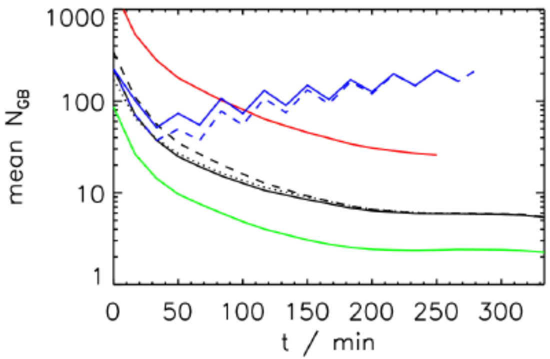
Due to dilution, the cloud area increases and thus the SIP number per grid box N_{GB} decreases

Additional option: SIP splitting -> increase SIP number during simulation



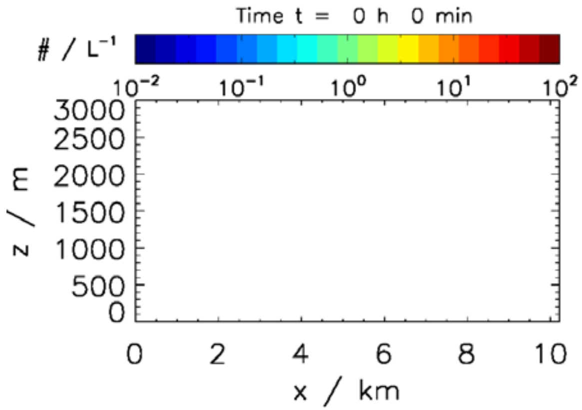
Convergence issue: Deposition and sedimentation





SIP number

Convergence issue: Nucleation



Simulation with homogenous nucleation

Nucleation highly non-linear: the number of nucleating ice crystals depends sensitively on the cooling rate

Nucleation implementation

Physics: Number of nucleated ice crystals m_{nuc} in a grid box:

$$m_{nuc} = J_f(a_w) \ * \ V_{a,i} \ * \ n_{a,i} \ * \ \Delta t_{nuc} \ * \ V_{GB}$$

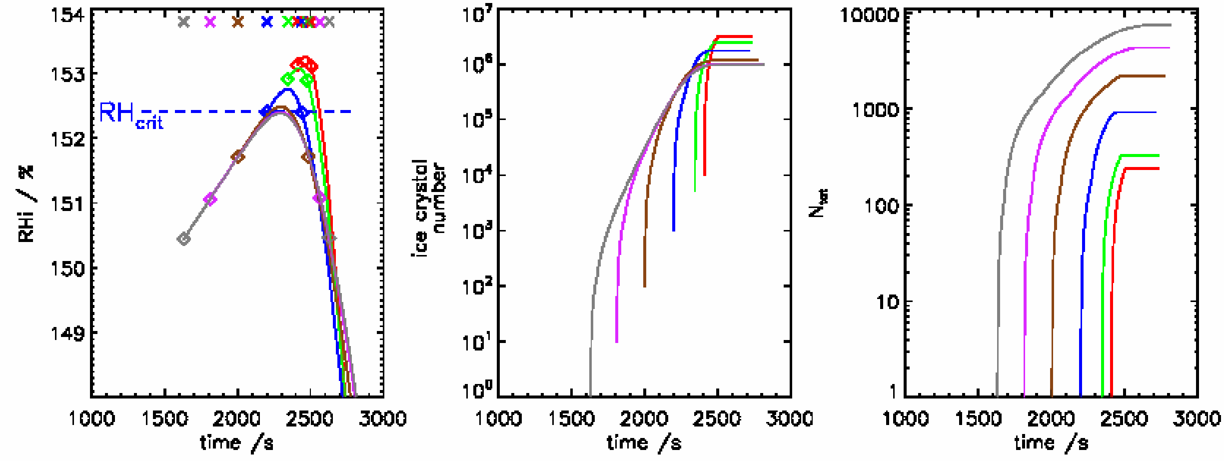
- Nucleation rate $J_f(a_w)$: depends on relative humidity
- $V_{a,i}$ volume of one aerosol in bin i
- $n_{a,i}$ number concentration of aerosols in bin i
- Nucleation timestep Δt_{nuc}
- Grid box volume V_{GB}

Implementation: SIP generation condition $m_{nuc} > m_{min}$

Stochastic nucleation implementation

Variation of m_{min} in box model simulations

RH_i | N Ice crystal | N SIP



Small m_{min}
Medium m_{min}
Large m_{min}

SIP generation condition $m_{nuc} > m_{min}$ retards ice crystal formation!!

Convergence issue: Nucleation

1. **Stochastic nucleation implementation**
2. SIP merge operation
3. Technical implementation

Stochastic nucleation implementation

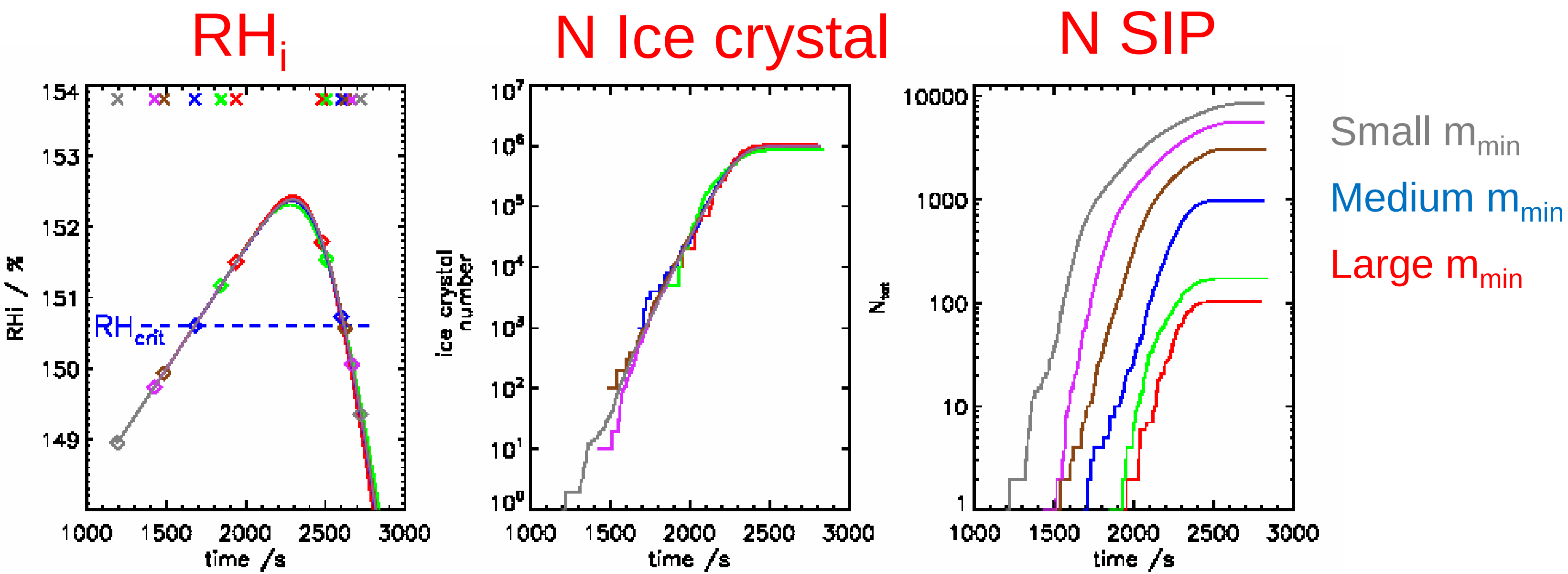
SOLUTION

If $m_{nuc} > m_{min:}$ generate SIP with $m_{sim} = m_{nuc}$ (as before)

If $m_{nuc} < m_{min}$:
generate SIP with $m_{sim} = m_{min}$ with probability $P_{SIP} = m_{nuc} / m_{min}$

Add stochastic component to nucleation implementation

Stochastic nucleation implementation

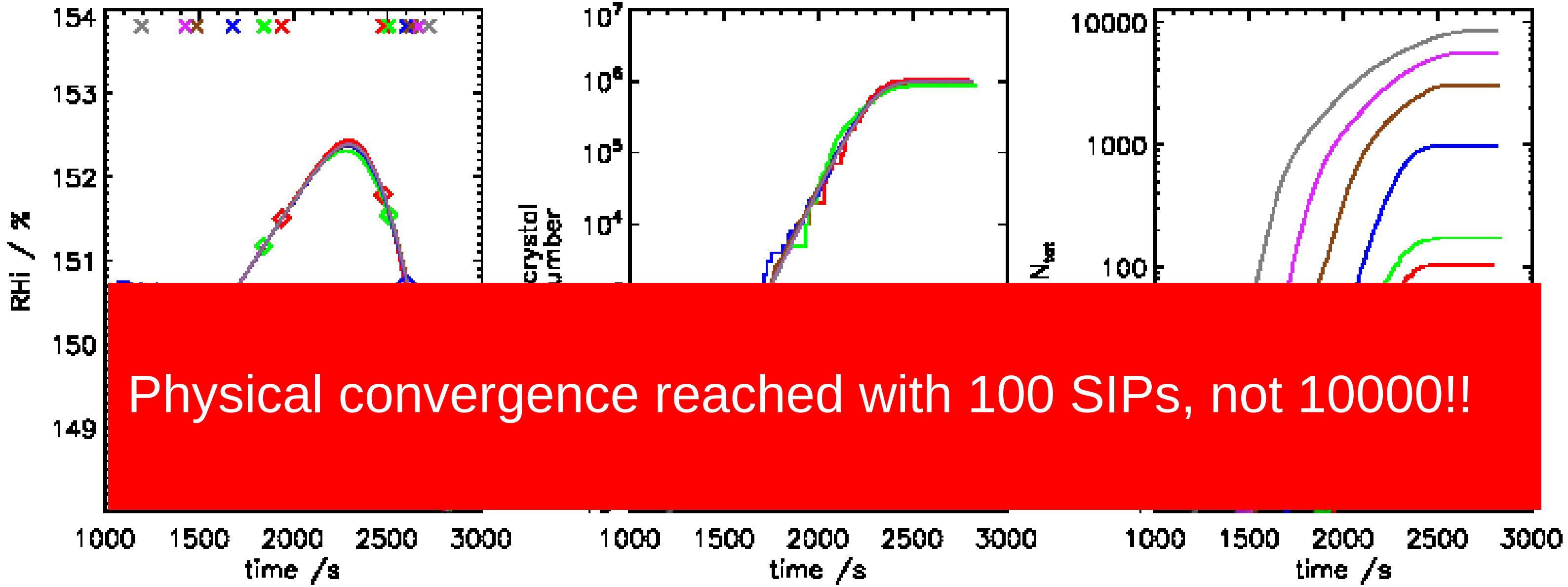


Stochastic component removes sensitivity to numerical parameter m_{min} !!

Stochastic nucleation implementation

Ice crystal

SIP



Physical convergence reached with 100 SIPs, not 10000!!

Convergence issue: Nucleation

1. Stochastic nucleation implementation
2. **SIP merge operation**
3. Technical implementation

SIP merge operation

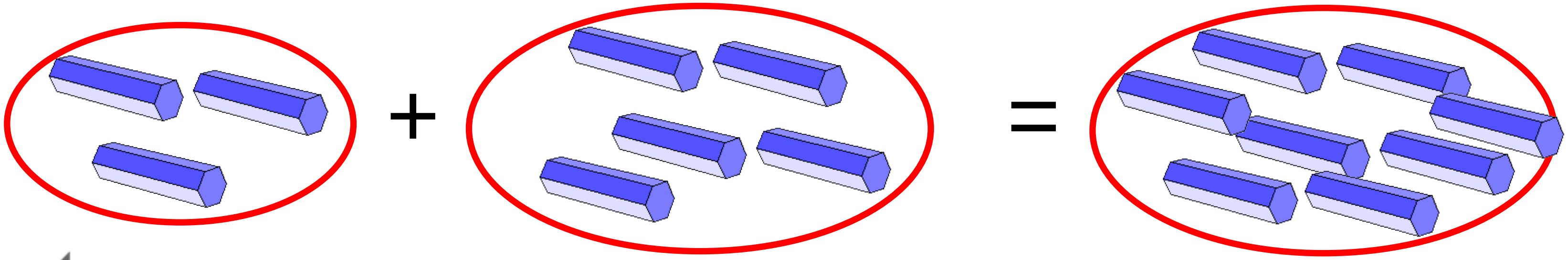
Deposition/sublimation and sedimentation are well resolved with few SIPs.

Operation SIPMERGE:
Merge two similar SIPs (position, radius) into one SIP with

SIP1
$m_{sim,1} = 3$ ice crystals

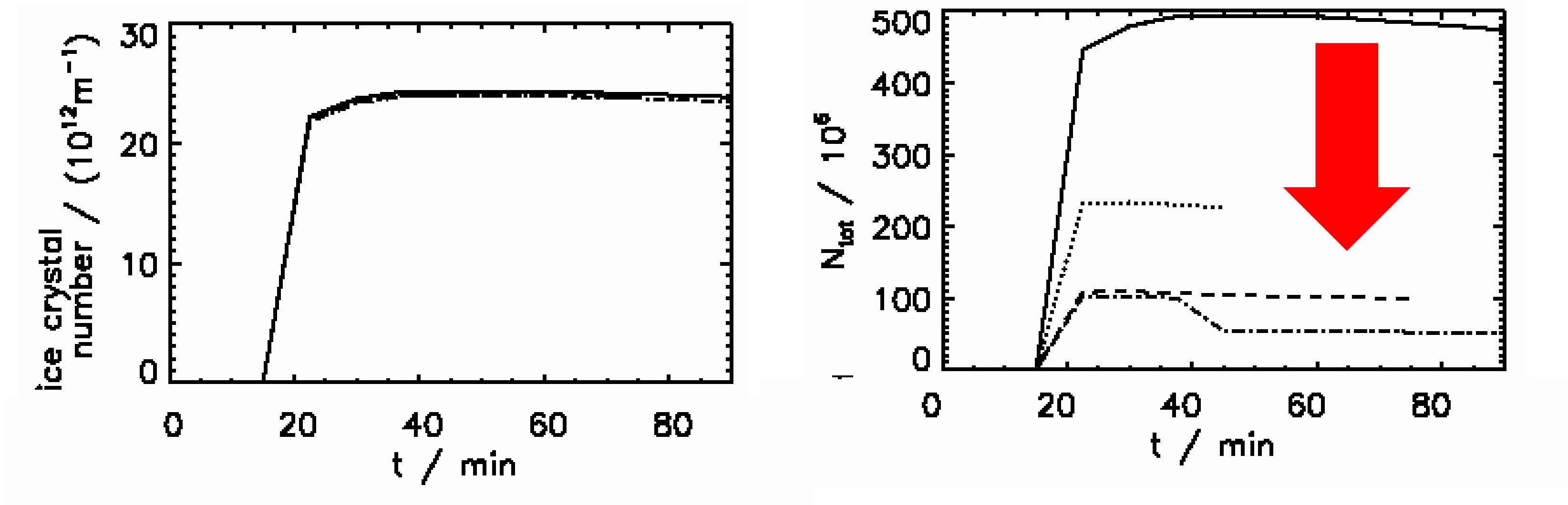
SIP2
$m_{sim,2} = 5$

SIPnew
$m_{sim,new} = m_{sim,1} + m_{sim,2}$



SIP merge operation

Application of SIPMERGE further reduces SIP number



Convergence issue: Nucleation

1. Stochastic nucleation implementation
2. SIP merge operation
3. **Technical implementation**

LCM implementation

First version of LCM implementation written in F77.
Static memory allocation of SIP data very memory-inefficient!!

- A-priori guess for maximum number of SIPs per processor and per grid box.
- Inefficient data structure to keep track to which grid box a SIP belongs.
- But number of SIPs in each GB varies a lot.

LCM implementation

Dynamic SIP memory allocation using singly linked lists

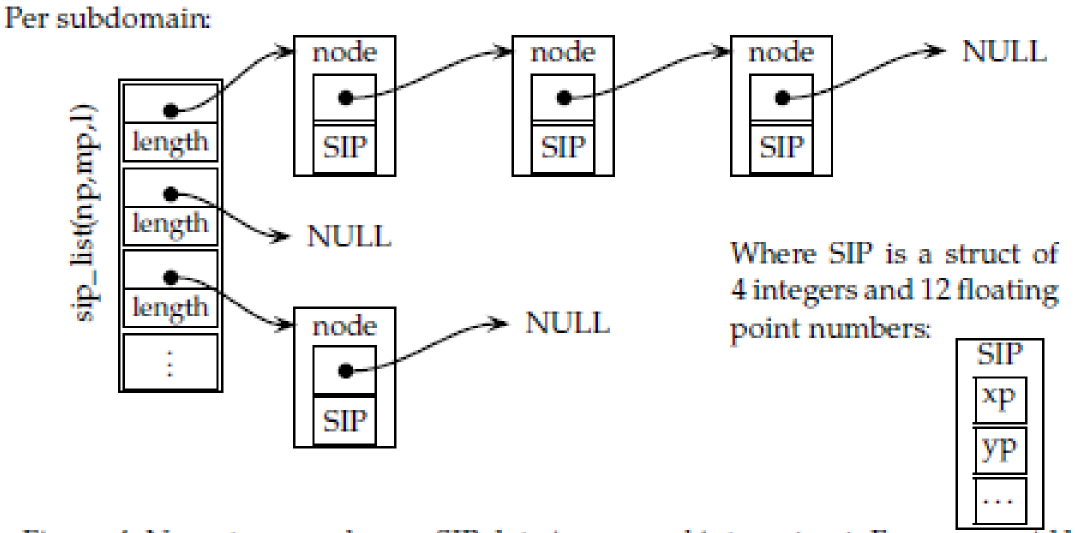
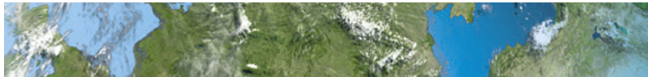


Figure 4: New storage scheme: SIP data is grouped into a *struct*. For every grid box there is a separate linked list which stores those SIP *structs*. The *sip_list* array contains a pointer to the head of each linked list.

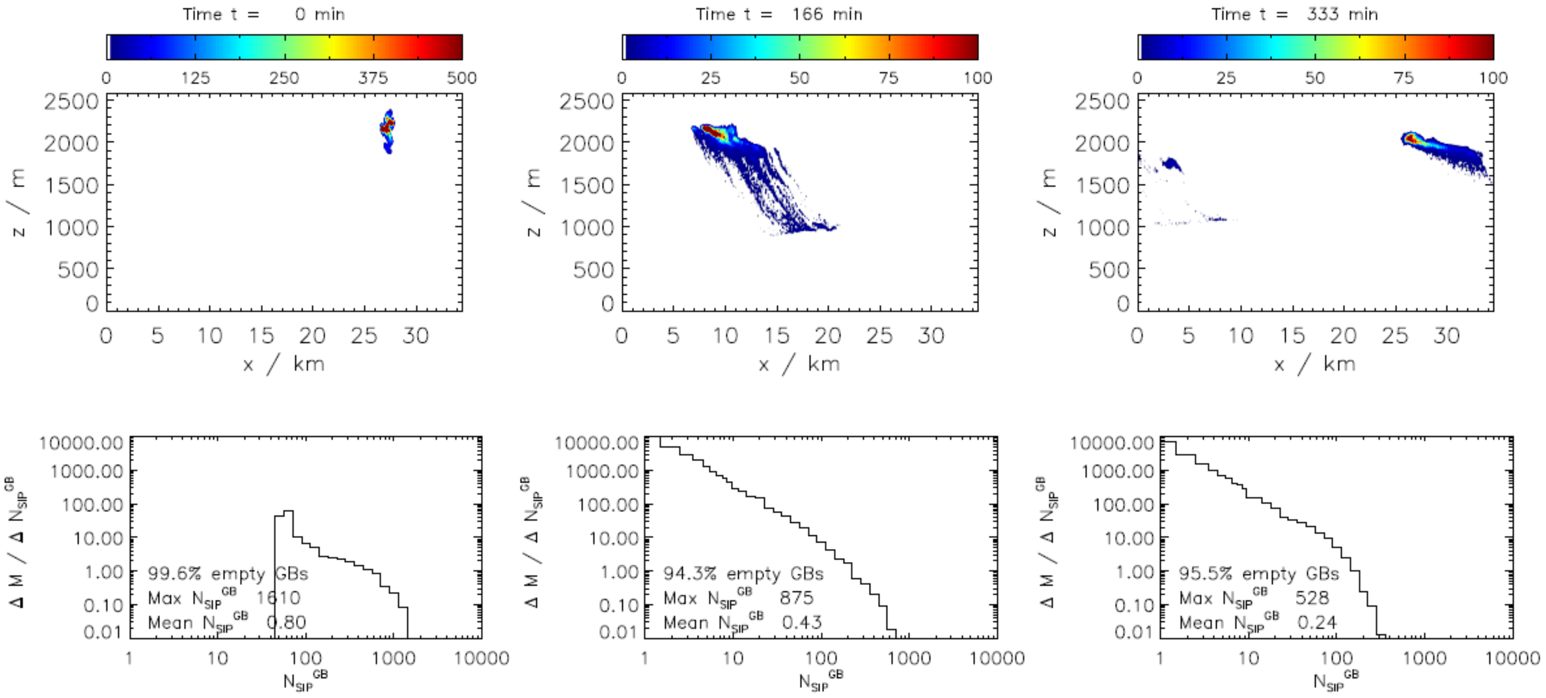
No more memory wasting

B. Stegmaier, Oct 2013, master thesis CompSci

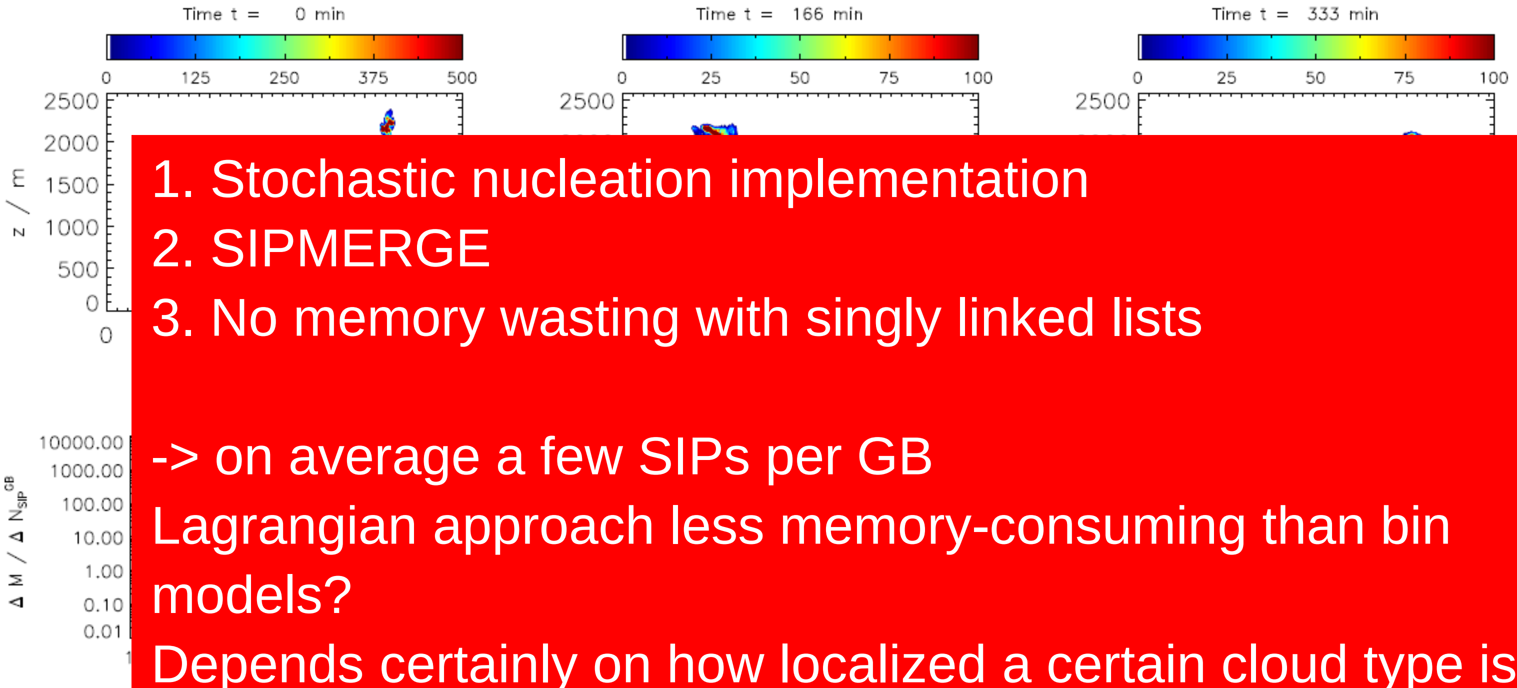


SIP number statistics

$N_{SIP,GB}$



LCM implementation



1. Stochastic nucleation implementation
2. SIPMERGE
3. No memory wasting with singly linked lists

-> on average a few SIPs per GB

Lagrangian approach less memory-consuming than bin models?

Depends certainly on how localized a certain cloud type is

Figure 2: A simulated contrail cirrus cloud after 0 min, 166 min and 333 min. The upper panel shows the number of SIPs per grid box $N_{\mathrm{SIP}}^{\mathrm{GB}}$ over a 2D cross-section. Colorbars do not extend to the maximum $N_{\mathrm{SIP}}^{\mathrm{GB}}$ value. The frequency of occurence of a certain $N_{\mathrm{SIP}}^{\mathrm{GB}}$ value can be read from the histograms in the lower panel. Only non-empty grid boxes are taken into account, as $N_{\mathrm{SIP}}^{\mathrm{GB}}$ is zero for over 94% of all grid boxes.

Conclusion

- Lagrangian ice microphysical module LCM presented (Sölch & Kärcher, QJRMS, 2010): Explicit aerosol and ice microphysics fully coupled to EULAG

- Methodological benefits demonstrated

- Convergence analyses (Unterstrasser & Sölch, GMD, 2014):
  - Adaptive control of SIP number: splitting and merging
  - Reduction of SIP number by stochastic nucleation implementation

- Applicability demonstrated (Unterstrasser et al, ACP, 2014):
  3D-simulations with millions of SIPs can be used for parametric studies

Acknowledgement

The simulations were carried out at the high performance computing facilities of the DKRZ in Hamburg.

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CONCLUSION=CONtrailCLUsterSimulatION

Thanks to meeting organizers for the invitation!

List of LCM publications

Model development: Sölch & Kärcher, QJRMS, 2010; Unterstrasser & Sölch, GMD, 2014

Cirrus simulations: Sölch & Kärcher, QJRMS, 2011; Kärcher, Dörnbrack & Sölch, JAS, 2014, Unterstrasser & Sölch, TAC3-Proc, 2013

Contrail simulations: Unterstrasser et al, ACP, 2014; Unterstrasser, JGR, 2014; Unterstrasser & Görsch, JGR, 2014